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COMBUSTION RESEARCH FACILITY
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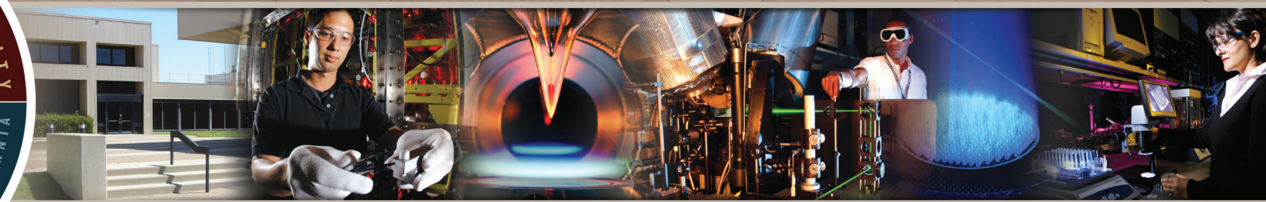

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Introducing the Engine Combustion Network

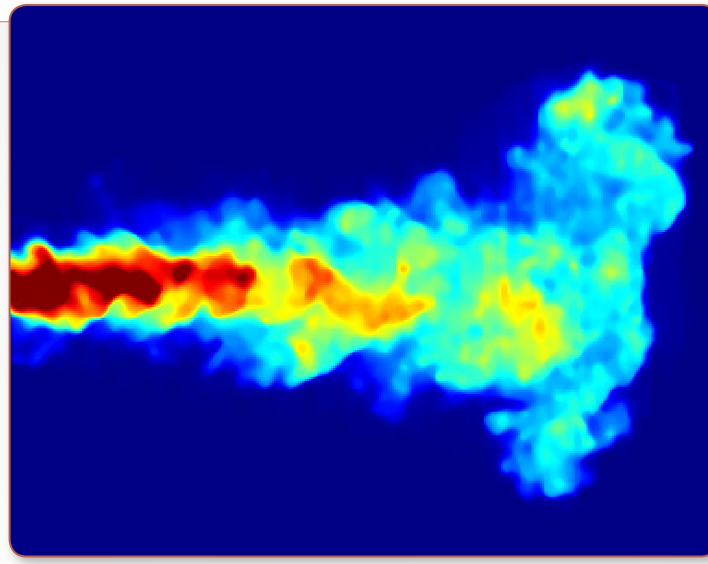

Figure 1. *Rayleigh scattering is used to instantly measure experimental mixture fraction, thus providing a quantitative comparison of spray evaporation and mixing at a high-temperature, high-pressure condition. Quantitative comparisons such as this one can be used to improve CFD models of realistic engine conditions.*

Researchers at the CRF have initiated a new collaborative effort for engine combustion research and modeling. The collaboration began when Lyle Pickett, a member of the Engine Combustion Research department, along with student interns Andrew Brough and Paul Nyholm, developed the Engine Combustion Network (ECN), a Web site (http://public.ca.sandia.gov/ECN/) featuring an Internet data archive library.

The ECN Web site is publicly accessible and contains data from well-documented diesel-spray experiments in engine-type conditions. For example, CRF researchers Pickett and Dennis Siebers (now managing Sandia's engine combustion research program), along with other visiting researchers, performed research using an optically accessible chamber designed to operate at pressures as high as 350 bar with controlled gas temperatures as high as 1400 K prior to spray injection. The ECN Web site contains data collected from this facility over the span of many years.
Since the launch of the ECN Web site, the project has attracted significant attention from the engine modeling community. Figure 1 shows that quantitative comparisons of spray evaporation and mixing at high-temperature, high-pressure conditions are now possible, providing opportunities to improve computational-fluid-dynamics (CFD) models of realistic engine conditions. The ECN dataset includes both reacting and nonreacting data, such as liquid and vapor penetration versus time, liquid length, ignition delay and pressure-rise rate, lift-off length, and quantitative soot volume fraction. This dataset is especially suitable for detailed CFD model validation because it contains many different types of experimental results collected under the same operating conditions.

Many scientists have responded favorably to the ECN initiative and are interested in collaborating on future research to advance the science of engine combustion.

(Continued on page 2)

Explosive detection using ion mobility spectrometry

Ion mobility spectrometry (IMS) is a very common sensing method deployed today for early detection of explosive compounds. A hallmark of IMS is that the fundamental operating principles are quite simple; the sensing device requires just a few components, all of which can be easily miniaturized. Operating at atmospheric conditions, these devices work by initially ionizing a neutral gas sample, then spatially separating the product ions by pushing them down a drift region under the influence of an electric field. The drifting ions collide onto a collector plate, rendering a unique ion-arrival waveform that is specific to the chemical species originally present in the sample.

Traditional IMS instruments achieve ionization through a series of ion–molecule reactions initiated by a radioactive alpha or beta emitter, typically ^{241}Am or ^{63}Ni, respectively. These sources, while robust and operationally simple, face severe regulatory barriers with regard to transportation and use. The difficulty of working within these regulations has prompted the development of alternative ionization schemes such as corona discharge and laser-induced ionization. The appeal of the latter

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Newsletter

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To this end, the ECN working group has identified a few experimental conditions that will be the focus of modelers and experimentalists who wish to collaborate in this effort.

The first target experimental condition is a low-temperature combustion condition relevant to a compression ignition engine using moderate exhaust gas recirculation (in-cylinder conditions of 900 K, 60 bar, 22.8 kg/m^{3,} and 15% oxygen at the time of fuel injection). The injector conditions are a common rail fuel injector with the following specifications: 1500-bar injection pressure, KS1.5/86 nozzle, 0.090-mm orifice diameter, and n-dodecane fuel at a temperature of 363 K. Research using the same injection system is made by possible by Robert Bosch LLC, which has donated a set of identical common-rail fuel injectors to users of the ECN. Participants in the ECN from around the world will apply advanced diagnostics at their own respective facilities to generate a comprehensive dataset at these operating conditions. Initial participants include CRF researchers and experimental groups at Argonne National Laboratory, Michigan Technological University, IFP (the French Petroleum Institute), the Polytechnic University of Valencia, Seoul National University, and Meiji University. Each ECN participant will make a significant effort to verify the ambient and injector boundary conditions at their own facilities. By working together in the ECN, all groups will benefit by sharing advanced diagnostics and boundary condition information one with another.

The ECN project is modeled after the Turbulent Non-premixed Flame (TNF) workshop, which was also initiated by the CRF. Years of quantitative experimental effort on well-defined flames (e.g., "Flame D") in the TNF workshop have created a standard library of data for computational comparison. The ECN seeks to generate a similar database for engine conditions.

In addition to experimental data, advanced CFD modeling results will be made available on the ECN Web site. These high-end, computationally intensive models could be used for comparison with low-level models. CFD modeling results with different grid resolution and fidelity are demonstrated in Figure 2.

The overall goal of the ECN effort is to facilitate the validation of computational models at conditions appropriate for engines. The improved models can then be used by industry to optimize the designs for advanced high-efficiency, low-emission engines. Supporting the development of these advanced engines is central to the mission of the DOE Office of Vehicle Technologies, which is sponsoring the development of the ECN and much of the research at the participating U.S. institutions.

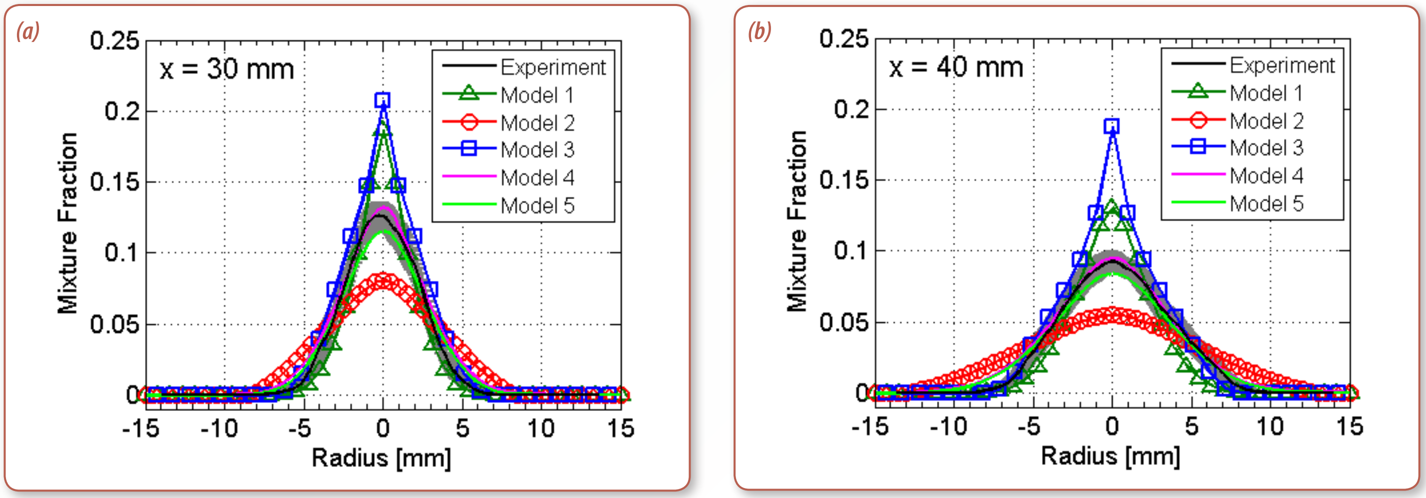


Figure 2. *Ensemble-averaged mixing measurements, as compared to various CFD predictions, at axial distances of (a) 30 mm and (b) 40 mm from the injector in the "baseline n-heptane" experimental condition. (Ambient: 1000 K, 14.8 kg/m3, 42 bar. Injector: common rail, 0.100-mm nozzle, 1540 bar, n-heptane fuel.) The gray border regions indicate experimental uncertainty.*

Combustion Research Facility Visitor Program

These visitors have recently completed their tenures at the Combustion Research Facility.

Emma Stewart, a visitor from the University of Strathclyde in Glascow, U.K., recently completed her doctoral thesis, "Modeling and Analysis of Small-Scale Fuel Cells for Distributed Generation," under the direction of Andy Lutz of the Hydrogen and Combustion Technologies Organization. In the course of her research, she collaborated on a test bed for the integration and validation of hydrogen generation, storage, and use in a real-world environment at Kahua Ranch, located on the Big Island of Hawaii. She also led an effort, as part of the International Energy Agency Annex 18 analysis task, to perform an analysis of the control system strategy of the "Hydrogen from the Sun/Ecological House" project located in Brescia, Italy. In this project, two control algorithms were developed for the house using a fuzzy logic and an adaptive control strategy.

Sang Min Lee was a visiting researcher from the Korea Institute of Machinery & Materials (KIMM) for a one-year period (February 2008 to March 2009). He joined Sandia researchers Tim Williams, Ethan Hecht, and Christopher Shaddix in collecting data on the effects of coal rank and gas temperature on the burning rate of pulverized coal during oxy-fuel combustion, a new technology for producing electricity from coal with near-zero emissions of CO_2. The results from these measurements were presented at the U.S. National Combustion Meeting in May and an international coal research meeting in June, and formed the basis of a journal paper that is in preparation.

Ulf Aronsson, a PhD student from Lund Institute of Technology in Sweden, completed a three-month visit to the CRF in early February. Ulf worked with Paul Miles and Isaac Ekoto in the Automotive Diesel Combustion Laboratory, performing in-cylinder imaging of the spatial distributions of unburned hydrocarbons and CO in an engine operating in a low-temperature, partially premixed combustion regime. The study focused on clarifying the impact of variations in squish height and fuel spray targeting on combustion efficiency.

Sanghoon Kook is a post-doc who worked with Lyle Pickett to conduct investigations of diesel engine fuel-air mixing, combustion, and emissions processes using various laser-based diagnostics. Their research expanded the science base regarding the use of advanced fuel injection and low-temperature combustion strategies for meeting future emissions requirements.

Continuing a long-running collaboration between Sandia Laboratories and the Technical University of Darmstadt, Germany, **Frederik Fuest** visited the Turbulent Combustion Laboratory to work with Rob Barlow and Bob Harmon on two projects aimed at extending capabilities for multiscalar measurements in flames at both institutions. The first involved developing a hybrid approach for analyzing Raman scattering measurements that combined aspects of distinct methods used by the two groups. The second project included measurements of polarized and depolarized signals from heated flows and laminar jet flames of ethane, ethylene, propane, and dimethyl ether. These measurements are a precursor of experiments on turbulent flames of these same fuels and implementation of the polarization separation and subtraction technique for single-shot Raman scattering measurements in turbulent flames with high levels of interference from hydrocarbon fluorescence or flame luminosity.

Will Colban completed three years as a post-doc working with Paul Miles in the Automotive Diesel Combustion Laboratory. During this time, Will was instrumental in commissioning a new, optically accessible engine based on a General Motors design, performing multiple studies clarifying the impact of engine operating conditions on the efficiency and emissions characteristics of low-temperature diesel combustion regimes, and developing and applying the capability of making full-field velocity measurements within the complex geometry of the diesel combustion chamber. Will has moved to a position with Alstom, SA, outside of Zurich, Switzerland, where he is responsible for developing optically based measurement techniques to assist in product development.

Sandians and members of the public "test drive the future" at the Hydrogen Road Tour


TEST-DRIVE THE FUTURE

Sandia National Laboratories

LIVERMORE

On May 28, join Sandia National Laboratories, the City of Livermore, and Livermore Downtown Inc. to test-drive (or ride) hydrogen-powered fuel cell vehicles from leading automakers! Meet the members of the California Fuel Cell Partnership, and talk to Sandia researchers and other engineers who work on the vehicles. *The public is welcome!*

Fuel cell vehicles have the potential to provide the range, high efficiency, rapid refueling, and performance consumers expect, along with zero tailpipe emissions and dramatically reduced greenhouse gas emissions. Come and see how close these vehicles are to commercialization, learn how to fill a fuel cell vehicle with hydrogen, and find out how fuel cells fit into Livermore's clean-air future.

HYDROGEN road tour 09

Who: Sandia National Laboratories, the City of Livermore, and Livermore Downtown Inc. in collaboration with the California Fuel Cell Partnership
What: Showcase and public "ride-and-drive" of hydrogen-powered fuel cell vehicles
Where: Downtown Livermore (the parking lot between First St. and Railroad Ave. in the old Lucky supermarket location)
When: Thursday, May 28, 2009, 11 a.m. to 1 p.m.

Contact:
Mike Janes
Sandia National Laboratories
(925) 294-2447
mejanes@sandia.gov

Clean. Quiet. Different.
Hydrogen-powered fuel cell vehicles.

ZERO EMISSION

Sandians and over 100 members of the public interested in learning first-hand about how hydrogen fuel cell-powered vehicles might be part of our transportation future took part in the "Hydrogen Road Tour," which made a stop in downtown Livermore on Thursday, May 28. The Road Tour brought out a diverse crowd that included scientists, auto enthusiasts, and the simply curious.

As part of the event – organized by Sandia, the City of Livermore, and Livermore Downtown, Inc. on behalf of the California Fuel Cell Partnership (CAFCP) – a dozen hydrogen fuel cell vehicles were stationed between First St. and Railroad Ave. Visitors had an opportunity to view, refuel, and even test drive or ride in the vehicles. In addition, members of CAFCP and engineers from leading automakers including Honda, Toyota, Nissa, Volkswagen, and GM (plus Sandia researchers) were on hand to talk about commercialization of the vehicles and hydrogen research projects.

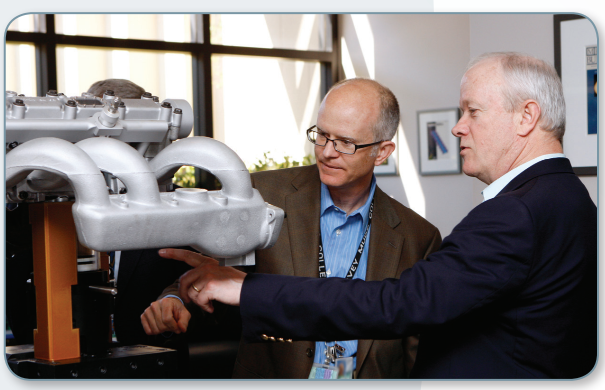
"Every major automaker is working on hydrogen-powered vehicles, and California has more fuel cell vehicles and hydrogen stations than any other region of the world," said Jay Keller, manager of the Hydrogen & Combustion Technology department, whose relationship with the CAFCP led to Livermore's selection as a stop on this year's tour. "This event offers a terrific showcase for some of those vehicles and gives people a unique opportunity to see how they look and perform."

Take our daughters and sons to work day 2009

Sandia/California's annual Take Our Daughters and Sons to Work Day occurred this year on April 23, allowing Sandia employees and contractors to invite children to visit their workplace to learn more about their hosts' work and Sandia's mission. This event is more than a career day; it is also an avenue to encourage students to pursue science, technology, engineering, and math careers. Members of the CRF hosted several fascinating demonstrations. Optical properties including refraction, reflection, and wavelength interaction were explored using the laser jello apparatus. The dilatant properties of non-Newtonian fluids were demonstrated via a large pool of "oobleck" (cornstarch and water), which flows easily with a gentle push, but resists more and more the harder you push. Participants also had the opportunity to assemble a LEGO NXT robot, write a simple computer program to control its movements, and then test the results in a cereal-box obstacle course.

Future scientists assemble a robot prior to field-testing. (Photo by Randy Wong)

Congressman Jerry McNerney visits the CRF



Andy McIlroy (left) shows Jerry McNerney an optical engine developed at Sandia for combustion research. (Photo by Randy Wong)

On Monday, April 20, Congressman Jerry McNerney (Democrat, 11th District) paid a visit to Sandia/California's Combustion Research Facility to learn about our energy programs. Terry Michalske, Andy McIlroy, and Karen Scott hosted the visit. While at Sandia, McNerney spent time in the Combustion Chemistry Laboratory, where he spoke with Craig Taatjes; the Turbulent Combustion Laboratory, where he met with Rob Barlow and Joe Oefelein; and the Advanced Fuels Laboratory.

Prior to winning his seat in 2006, McNerney worked as a contractor at Sandia/New Mexico and had a long career in wind energy, consulting for PG&E, FloWind, and the Electric Power Research Institute, Inc. McNerney has many congressional assignments, including the Energy and Commerce Committee, which is particularly relevant to Sandia. McNerney's district, which touches Alameda, Contra Costa, and San Joaquin counties, includes the cities of Danville, Dublin, Lodi, Manteca, Pleasanton, San Ramon, and Tracy.

Explosive detection (cont.)

(Continued from page 1)

method is increasing because lasers can be designed to operate over particular wavelength ranges corresponding to the absorption features of a given molecule or molecular class, thereby increasing the specificity of the ionization process. This level of selectivity cannot be achieved with corona discharge or the classic radioactive sources because those ionization methods are inherently indiscriminate.

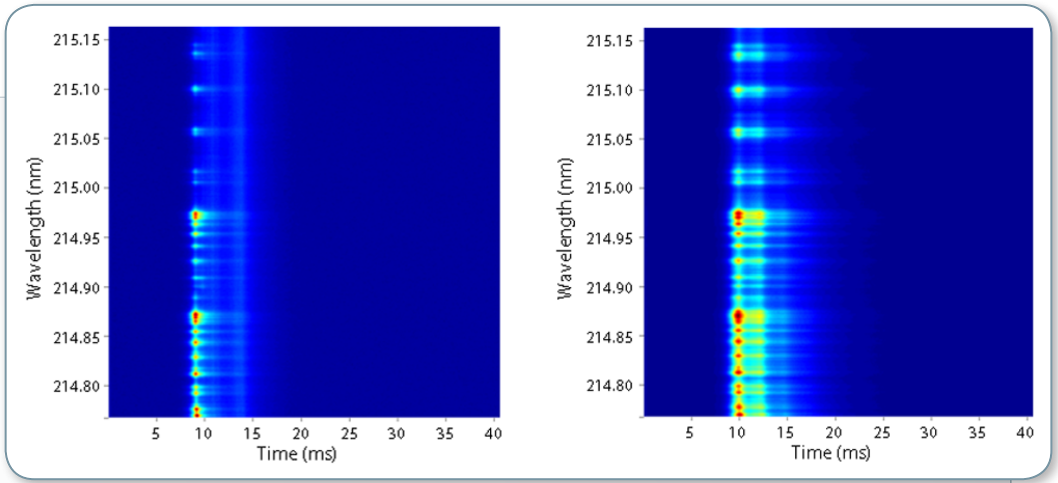


__Figure 1.__ The plots display the unique wavelength-dependent IMS traces of (a) 2, 4–dinitrotoluene and (b) nitrobenzene. Ion drift time is denoted on the horizontal axis and excitation wavelength on the vertical axis. Red areas signify signal maximums and blue areas represent little or no signal.

Recently, CRF researchers Thomas A. Reichardt and Jeffrey M. Headrick have coupled laser-induced ionization with IMS technology to detect ionic photofragements of the explosive surrogate 2, 4-dinitrotoluene and nuisance-compound nitrobenzene. Similar to common organic explosives (TNT, RDX, PETN, and HMX), these compounds contain the all-important NO_2 functional group; however, they are much safer to handle and easier to use than the organic explosives.

Using only a single laser centered at 215 nm, which corresponds to the NO $A^2\Sigma^+ \;\; X^2\Pi$ (1,0) transition, a four-photon excitation scheme is executed:

$$R - NO_2 \xrightarrow{2hv} R + 0 + NO\,(X^2\Pi)$$

$$NO\,(X^2\Pi) \xrightarrow{hv} NO\,(A^2\Sigma^+) \xrightarrow{hv} NO^+ + e^-$$

yielding NO^+ as the primary detectable photofragment. This wavelength range is appealing because it can be generated by frequency quintupling Nd- and Yb-doped lasers, an integral component necessary for the development of a compact, portable laser-based IMS system.

Tuning through the various laser excitation/ionization wavelengths increases the dimensionality of the IMS detection method. Traditional IMS measurements yield only a single temporally resolved ion-arrival waveform; however, with laser-induced ionization each IMS trace is identified with a unique wavelength "stamp." This is demonstrated in Figure 1. False-color maps depict the wavelength-dependent IMS signals for (a) 2, 4-dinitrotoluene and (b) nitrobenzene.

Figure 1 reveals that the two compounds yield unique fragmentation patterns when exposed to identical wavelengths of UV radiation. Extracting IMS slices along the horizontal axis (Figure 2) at the signal maximum (l = 214.872 nm) reveals detail not readily seen in the mapped data. Interestingly, the two compounds do not share a single ion-arrival time, an unexpected result because it is assumed that the target molecules generate at least one common photofragment, NO^+. It is believed that the discrepancies between the two IMS traces are due to the fact that each compound generates various photofragments, indicating that the product ions experience a diverse, local ionization environment. Because IMS measurements are conducted at atmosphere conditions it is expected that collisions between the product ions and neutral fragments will generate various ion–molecule complexes. The local ionization environment and subsequent clustering effects due to collisions are believed to lead to observed mobilities that are related to the parent compound, yielding species-specific IMS waveforms.

These results are encouraging and demonstrate that laser-induced ionization can render unique IMS traces. Other preliminary investigations reveal wavelength dependencies that depict the rotational energy distribution of the nascent NO^+ photofragment, which yields yet another observable phenomenon that aids in the detection of these compounds.

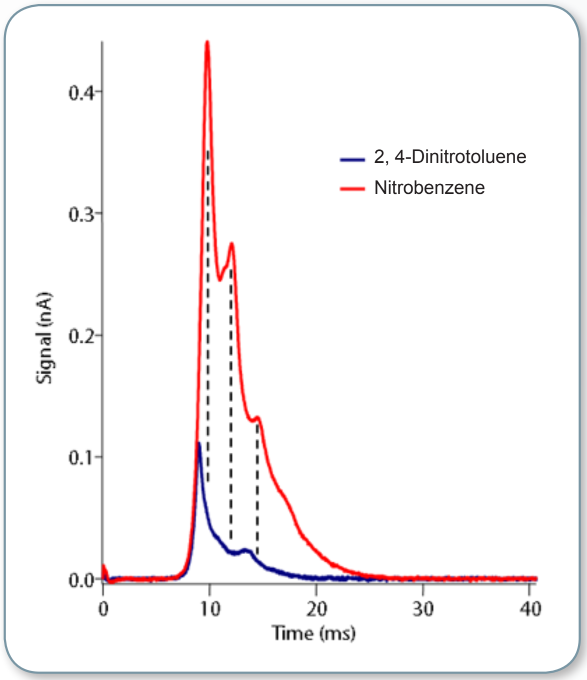
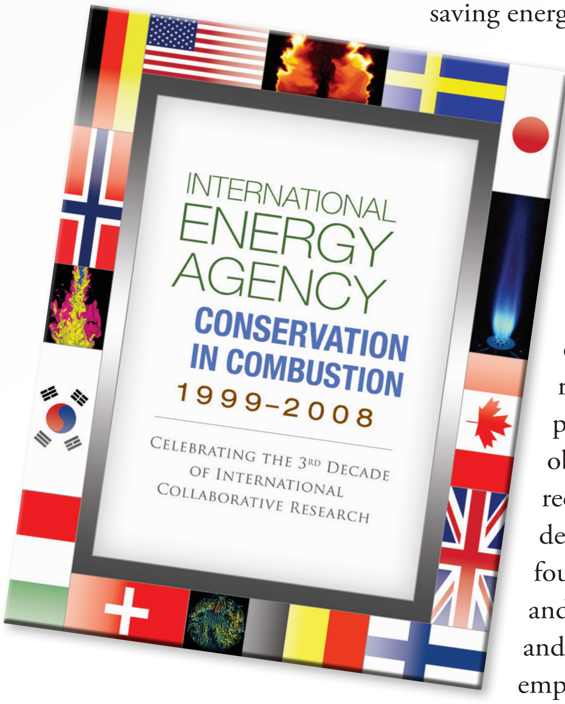


__Figure 2.__ IMS traces for 2, 4 – dinitrotoluene (blue) and nitrobenzene (red) when ionized at 214.872 nm. Collisions between the product ions and neutral fragments generate various ion-molecule complexes, which in turn yield species-specific IMS waveforms.

New combustion report released by the International Energy Agency

Conservation in Combustion, a document highlighting activities conducted during the past ten years under the International Energy Agency's (IEA's) Energy Conservation and Emissions Reduction in Combustion Implementing Agreement, was officially released to the Agreement's 12 member countries on April 28, 2009, at the Paris meeting of the Agreement's Executive Committee. Dennis Siebers, who manages the Engine Combustion department at the CRF, attended the meeting as one of two U.S. Executive Committee members. CRF retiree Bob Gallagher serves as the Agreement's Executive Secretary and oversaw the preparation and publication of the IEA report, which is available for download at http://ieacombustion.com/19992008anniversaryrpt.aspx.



The *Conservation in Combustion* report is a record of the Agreement's singular achievements in energy conservation and emissions reduction in combustion over the past 10 years, from 1999 to 2008. It also celebrates the third decade of international collaborative research devoted to saving energy and reducing pollution by increasing fundamental knowledge about combustion.

The IEA's Energy Conservation and Emissions Reduction in Combustion Implementing Agreement was formally organized in 1977 to accelerate the development of combustion technologies that reduce fuel consumption and lower pollutant emissions. The Agreement's objectives have been expanded in recent years to include research, development, and demonstration in four areas: fundamentals of combustion and advanced piston engine, gas turbine, and furnace technologies. The Agreement emphasizes industrial involvement to ensure that adequate attention is paid to industry needs and that technology is disseminated to the marketplace. Task sharing among member nations and personnel exchanges are employed to facilitate reaching the Agreement's goals.

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